1.4. Support Vector Machines

Support vector machines (SVMs) are a set of supervised learning methods used for classification, regression and outliers detection.

The advantages of support vector machines are:

- Effective in high dimensional spaces.
- Still effective in cases where number of dimensions is greater than the number of samples.
- Uses a subset of training points in the decision function (called support vectors), so it is also memory efficient.
- Versatile: different Kernel functions can be specified for the decision function. Common kernels are provided, but it is also possible to specify custom kernels.

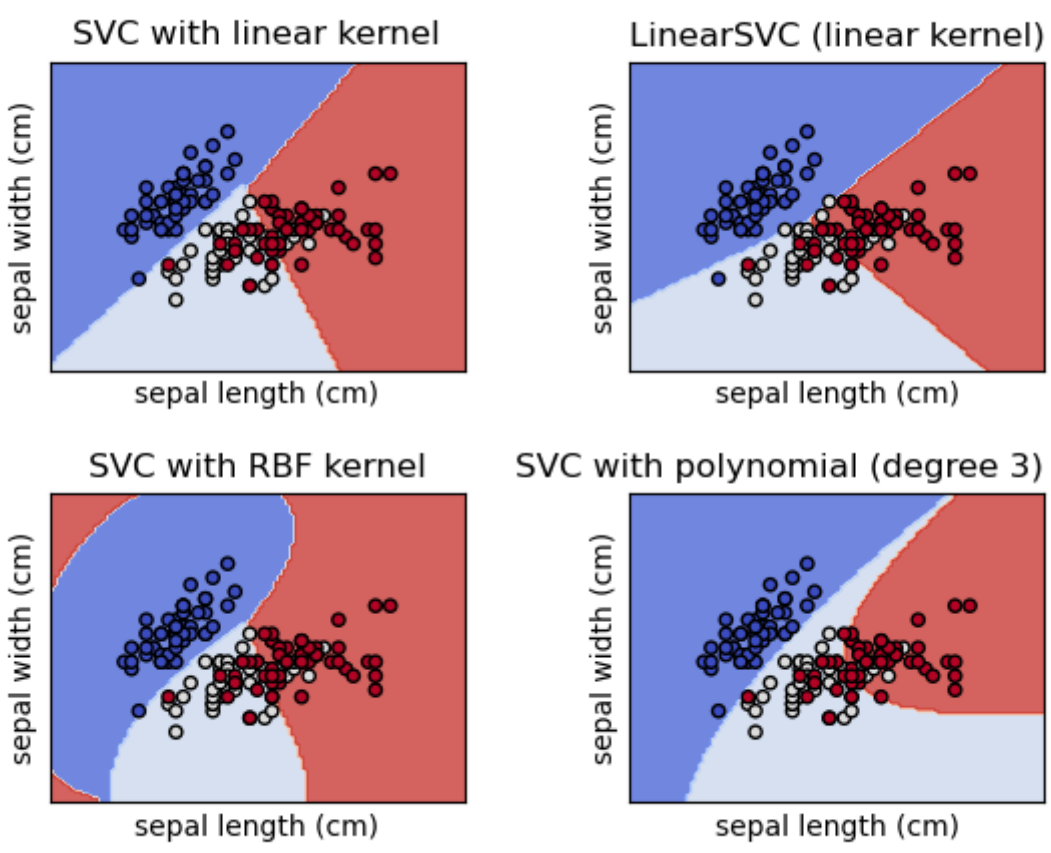
The disadvantages of support vector machines include:

- If the number of features is much greater than the number of samples, avoid over-fitting in choosing Kernel functions and regularization term is crucial.
- SVMs do not directly provide probability estimates, these are calculated using an expensive five-fold cross-validation (see Scores and probabilities, below).

The support vector machines in scikit-learn support both dense (`numpy.ndarray` and convertible to that by `numpy.asarray`) and sparse (any `scipy.sparse`) sample vectors as input. However, to use an SVM to make predictions for sparse data, it must have been fit on such data. For optimal performance, use C-ordered `numpy.ndarray` (dense) or `scipy.sparse.csr_matrix` (sparse) with `dtype=float64`.

1.4.1. Classification

`SVC`, **`NuSVC`** and **`LinearSVC`** are classes capable of performing binary and multi-class classification on a dataset.



`SVC` and **`NuSVC`** are similar methods, but accept slightly different sets of parameters and have different mathematical formulations (see section Mathematical formulation). On the other hand, **`LinearSVC`** is another (faster) implementation of Support Vector Classification for the case of a linear kernel. Note that **`LinearSVC`** does not accept parameter `kernel`, as this is assumed to be linear. It also lacks some of the attributes of **`SVC`** and **`NuSVC`**, like `support_`.

As other classifiers, **`SVC`**, **`NuSVC`** and **`LinearSVC`** take as input two arrays: an array `X` of shape `(n_samples, n_features)` holding the training samples, and an array `y` of class labels (strings or integers), of shape `(n_samples)`:

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```
>>> from sklearn import svm
>>> X = [[0, 0], [1, 1]]
>>> y = [0, 1]
>>> clf = svm.SVC()
>>> clf.fit(X, y)
SVC()
```

After being fitted, the model can then be used to predict new values:

```
>>> clf.predict([[2., 2.]])
array([1])
```

SVMs decision function (detailed in the Mathematical formulation) depends on some subset of the training data, called the support vectors. Some properties of these support vectors can be found in attributes `support_vectors_`, `support_` and `n_support_`:

```
>>> # get support vectors
>>> clf.support_vectors_
array([[0., 0.],
       [1., 1.]])
>>> # get indices of support vectors
>>> clf.support_
array([0, 1]...)
>>> # get number of support vectors for each class
>>> clf.n_support_
array([1, 1]...)
```

Examples:

- SVM: Maximum margin separating hyperplane,
- Non-linear SVM
- SVM-Anova: SVM with univariate feature selection,

1.4.1.1. Multi-class classification

SVC and **NuSVC** implement the “one-versus-one” approach for multi-class classification. In total, `n_classes * (n_classes - 1) / 2` classifiers are constructed and each one trains data from two classes. To provide a consistent interface with other classifiers, the `decision_function_shape` option allows to monotonically transform the results of the “one-versus-one” classifiers to a “one-vs-rest” decision function of shape `(n_samples, n_classes)`.

```
>>> X = [[0], [1], [2], [3]]
>>> Y = [0, 1, 2, 3]
>>> clf = svm.SVC(decision_function_shape='ovo')
>>> clf.fit(X, Y)
SVC(decision_function_shape='ovo')
>>> dec = clf.decision_function([[1]])
>>> dec.shape[1] # 4 classes: 4*3/2 = 6
6
>>> clf.decision_function_shape = "ovr"
>>> dec = clf.decision_function([[1]])
>>> dec.shape[1] # 4 classes
4
```

On the other hand, **LinearSVC** implements “one-vs-the-rest” multi-class strategy, thus training `n_classes` models.

```
>>> lin_clf = svm.LinearSVC(dual="auto")
>>> lin_clf.fit(X, Y)
LinearSVC(dual='auto')
>>> dec = lin_clf.decision_function([[1]])
>>> dec.shape[1]
4
```

See Mathematical formulation for a complete description of the decision function.

▶ **Details on multi-class strategies**

Examples:

- Plot different SVM classifiers in the iris dataset,

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1.4.1.2. Scores and probabilities

The `decision_function` method of **`SVC`** and **`NuSVC`** gives per-class scores for each sample (or a single score per sample in the binary case). When the constructor option `probability` is set to `True`, class membership probability estimates (from the methods `predict_proba` and `predict_log_proba`) are enabled. In the binary case, the probabilities are calibrated using Platt scaling [9]: logistic regression on the SVM's scores, fit by an additional cross-validation on the training data. In the multiclass case, this is extended as per [10].

Note: The same probability calibration procedure is available for all estimators via the **`CalibratedClassifierCV`** (see Probability calibration). In the case of **`SVC`** and **`NuSVC`**, this procedure is builtin in libsvm which is used under the hood, so it does not rely on scikit-learn's **`CalibratedClassifierCV`**.

The cross-validation involved in Platt scaling is an expensive operation for large datasets. In addition, the probability estimates may be inconsistent with the scores:

- the "argmax" of the scores may not be the argmax of the probabilities
- in binary classification, a sample may be labeled by `predict` as belonging to the positive class even if the output of `predict_proba` is less than 0.5; and similarly, it could be labeled as negative even if the output of `predict_proba` is more than 0.5.

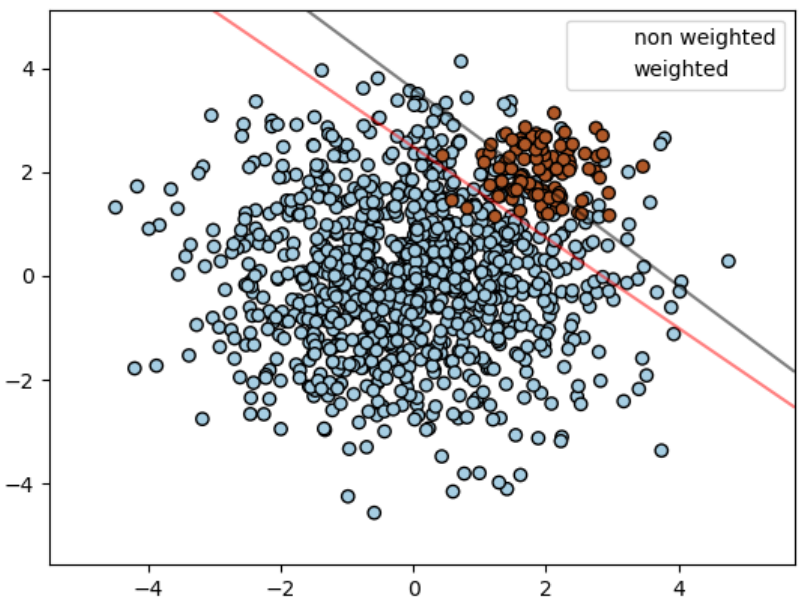
Platt's method is also known to have theoretical issues. If confidence scores are required, but these do not have to be probabilities, then it is advisable to set `probability=False` and use `decision_function` instead of `predict_proba`.

Please note that when `decision_function_shape='ovr'` and `n_classes > 2`, unlike `decision_function`, the `predict` method does not try to break ties by default. You can set `break_ties=True` for the output of `predict` to be the same as `np.argmax(clf.decision_function(...), axis=1)`, otherwise the first class among the tied classes will always be returned; but have in mind that it comes with a computational cost. See SVM Tie Breaking Example for an example on tie breaking.

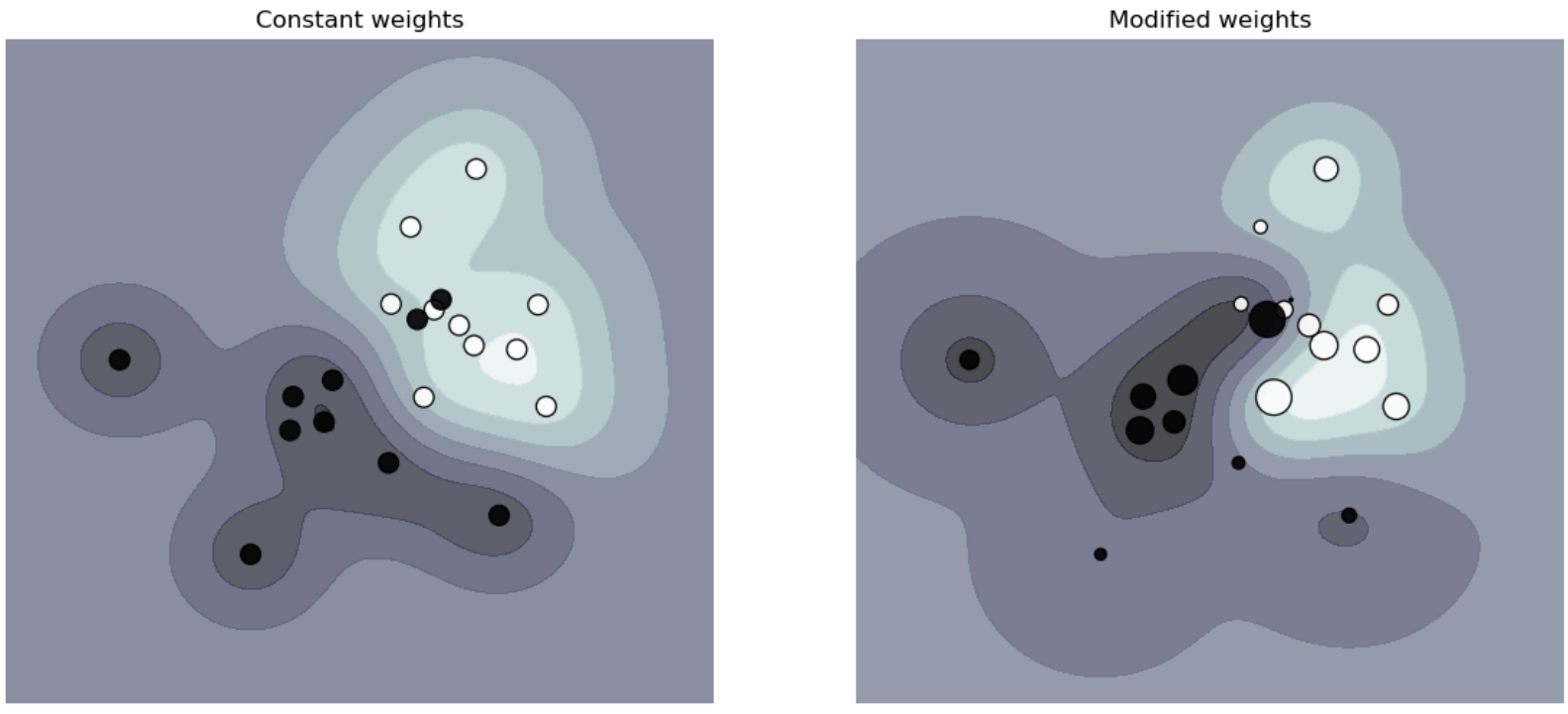
1.4.1.3. Unbalanced problems

In problems where it is desired to give more importance to certain classes or certain individual samples, the parameters `class_weight` and `sample_weight` can be used.

`SVC` (but not **`NuSVC`**) implements the parameter `class_weight` in the `fit` method. It's a dictionary of the form `{class_label : value}`, where value is a floating point number > 0 that sets the parameter `C` of class `class_label` to `C * value`. The figure below illustrates the decision boundary of an unbalanced problem, with and without weight correction.



`SVC`, **`NuSVC`**, **`SVR`**, **`NuSVR`**, **`LinearSVC`**, **`LinearSVR`** and **`OneClassSVM`** implement also weights for individual samples in the `fit` method through the `sample_weight` parameter. Similar to `class_weight`, this sets the parameter `C` for the i-th example to `C * sample_weight[i]`, which will encourage the classifier to get these samples right. The figure below illustrates the effect of sample weighting on the decision boundary. The size of the circles is proportional to the sample weights:



Examples:

- SVM: Separating hyperplane for unbalanced classes
- SVM: Weighted samples,

1.4.2. Regression

The method of Support Vector Classification can be extended to solve regression problems. This method is called Support Vector Regression.

The model produced by support vector classification (as described above) depends only on a subset of the training data, because the cost function for building the model does not care about training points that lie beyond the margin. Analogously, the model produced by Support Vector Regression depends only on a subset of the training data, because the cost function ignores samples whose prediction is close to their target.

There are three different implementations of Support Vector Regression: **SVR**, **NuSVR** and **LinearSVR**. **LinearSVR** provides a faster implementation than **SVR** but only considers the linear kernel, while **NuSVR** implements a slightly different formulation than **SVR** and **LinearSVR**. See Implementation details for further details.

As with classification classes, the fit method will take as argument vectors X, y, only that in this case y is expected to have floating point values instead of integer values:

```
>>> from sklearn import svm
>>> X = [[0, 0], [2, 2]]
>>> y = [0.5, 2.5]
>>> regr = svm.SVR()
>>> regr.fit(X, y)
SVR()
>>> regr.predict([[1, 1]])
array([1.5])
```

Examples:

- Support Vector Regression (SVR) using linear and non-linear kernels

1.4.3. Density estimation, novelty detection

The class **OneClassSVM** implements a One-Class SVM which is used in outlier detection.

See Novelty and Outlier Detection for the description and usage of OneClassSVM.

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1.4.4. Complexity

Support Vector Machines are powerful tools, but their compute and storage requirements increase rapidly with the number of training vectors. The core of an SVM is a quadratic programming problem (QP), separating support vectors from the rest of the training data. The QP solver used by the libsvm-based implementation scales between $O(n_{features} \times n_{samples}^2)$ and $O(n_{features} \times n_{samples}^3)$ depending on how efficiently the libsvm cache is used in practice (dataset dependent). If the data is very sparse $n_{features}$ should be replaced by the average number of non-zero features in a sample vector.

For the linear case, the algorithm used in **`LinearSVC`** by the liblinear implementation is much more efficient than its libsvm-based **`SVC`** counterpart and can scale almost linearly to millions of samples and/or features.

1.4.5. Tips on Practical Use

- **Avoiding data copy**: For `SVC`, `SVR`, `NuSVC` and `NuSVR`, if the data passed to certain methods is not C-ordered contiguous and double precision, it will be copied before calling the underlying C implementation. You can check whether a given numpy array is C-contiguous by inspecting its `flags` attribute.

  For `LinearSVC` (and `LogisticRegression`) any input passed as a numpy array will be copied and converted to the liblinear internal sparse data representation (double precision floats and int32 indices of non-zero components). If you want to fit a large-scale linear classifier without copying a dense numpy C-contiguous double precision array as input, we suggest to use the `SGDClassifier` class instead. The objective function can be configured to be almost the same as the `LinearSVC` model.

- **Kernel cache size**: For `SVC`, `SVR`, `NuSVC` and `NuSVR`, the size of the kernel cache has a strong impact on run times for larger problems. If you have enough RAM available, it is recommended to set `cache_size` to a higher value than the default of 200(MB), such as 500(MB) or 1000(MB).

- **Setting C**: `C` is `1` by default and it's a reasonable default choice. If you have a lot of noisy observations you should decrease it: decreasing C corresponds to more regularization.

  `LinearSVC` and `LinearSVR` are less sensitive to `C` when it becomes large, and prediction results stop improving after a certain threshold. Meanwhile, larger `C` values will take more time to train, sometimes up to 10 times longer, as shown in [11].

- Support Vector Machine algorithms are not scale invariant, so **it is highly recommended to scale your data**. For example, scale each attribute on the input vector X to [0,1] or [-1,+1], or standardize it to have mean 0 and variance 1. Note that the *same* scaling must be applied to the test vector to obtain meaningful results. This can be done easily by using a `Pipeline`:

  ```
  >>> from sklearn.pipeline import make_pipeline
  >>> from sklearn.preprocessing import StandardScaler
  >>> from sklearn.svm import SVC

  >>> clf = make_pipeline(StandardScaler(), SVC())
  ```

  See section Preprocessing data for more details on scaling and normalization.

- Regarding the `shrinking` parameter, quoting [12]: *We found that if the number of iterations is large, then shrinking can shorten the training time. However, if we loosely solve the optimization problem (e.g., by using a large stopping tolerance), the code without using shrinking may be much faster*

- Parameter `nu` in `NuSVC`/`OneClassSVM`/`NuSVR` approximates the fraction of training errors and support vectors.

- In `SVC`, if the data is unbalanced (e.g. many positive and few negative), set `class_weight='balanced'` and/or try different penalty parameters `C`.

- **Randomness of the underlying implementations**: The underlying implementations of `SVC` and `NuSVC` use a random number generator only to shuffle the data for probability estimation (when `probability` is set to `True`). This randomness can be controlled with the `random_state` parameter. If `probability` is set to `False` these estimators are not random and `random_state` has no effect on the results. The underlying `OneClassSVM` implementation is similar to the ones of `SVC` and `NuSVC`. As no probability estimation is provided for `OneClassSVM`, it is not random.

  The underlying `LinearSVC` implementation uses a random number generator to select features when fitting the model with a dual coordinate descent (i.e when `dual` is set to `True`). It is thus not uncommon to have slightly different results for the same input data. If that happens, try with a smaller `tol` parameter. This randomness can also be controlled with the `random_state` parameter. When `dual` is set to `False` the underlying implementation of `LinearSVC` is not random and `random_state` has no effect on the results.

- Using L1 penalization as provided by `LinearSVC(penalty='l1', dual=False)` yields a sparse solution, i.e. only a subset of feature weights is different from zero and contribute to the decision function. Increasing `C` yields a more complex model (more features are selected). The `C` value that yields a "null" model (all weights equal to zero) can be calculated using `l1_min_c`.

1.4.6. Kernel functions

The *kernel function* can be any of the following:

- linear: $\langle x, x' \rangle$.
- polynomial: $(\gamma \langle x, x' \rangle + r)^d$, where d is specified by parameter `degree`, r by `coef0`.
- rbf: $\exp(-\gamma \|x - x'\|^2)$, where γ is specified by parameter `gamma`, must be greater than 0.
- sigmoid $\tanh(\gamma \langle x, x' \rangle + r)$, where r is specified by `coef0`.

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Different kernels are specified by the `kernel` parameter:

```
>>> linear_svc = svm.SVC(kernel='linear')
>>> linear_svc.kernel
'linear'
>>> rbf_svc = svm.SVC(kernel='rbf')
>>> rbf_svc.kernel
'rbf'
```

See also Kernel Approximation for a solution to use RBF kernels that is much faster and more scalable.

1.4.6.1. Parameters of the RBF Kernel

When training an SVM with the *Radial Basis Function* (RBF) kernel, two parameters must be considered: `C` and `gamma`. The parameter `C`, common to all SVM kernels, trades off misclassification of training examples against simplicity of the decision surface. A low `C` makes the decision surface smooth, while a high `C` aims at classifying all training examples correctly. `gamma` defines how much influence a single training example has. The larger `gamma` is, the closer other examples must be to be affected.

Proper choice of `C` and `gamma` is critical to the SVM's performance. One is advised to use **`GridSearchCV`** with `C` and `gamma` spaced exponentially far apart to choose good values.

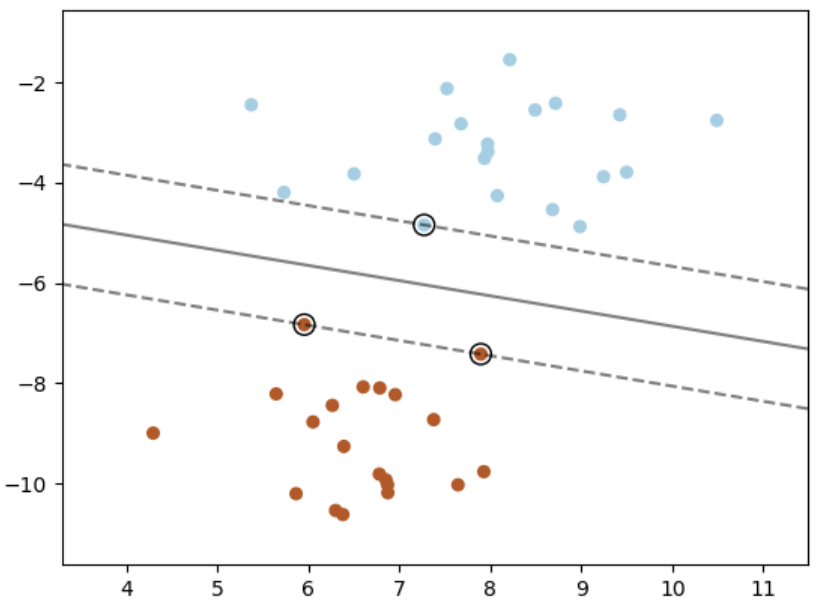
Examples:

- RBF SVM parameters
- Non-linear SVM

▶ **Custom Kernels**

1.4.7. Mathematical formulation

A support vector machine constructs a hyper-plane or set of hyper-planes in a high or infinite dimensional space, which can be used for classification, regression or other tasks. Intuitively, a good separation is achieved by the hyper-plane that has the largest distance to the nearest training data points of any class (so-called functional margin), since in general the larger the margin the lower the generalization error of the classifier. The figure below shows the decision function for a linearly separable problem, with three samples on the margin boundaries, called "support vectors":



In general, when the problem isn't linearly separable, the support vectors are the samples *within* the margin boundaries.

We recommend [13] and [14] as good references for the theory and practicalities of SVMs.

1.4.7.1. SVC

Given training vectors $x_i \in \mathbb{R}^p$, i=1,..., n, in two classes, and a vector $y \in \{1, -1\}^n$, our goal is to find $w \in \mathbb{R}^p$ and $b \in \mathbb{R}$ such that the prediction given by $\text{sign}(w^T \phi(x) + b)$ is correct for most samples.

SVC solves the following primal problem:

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$$\min_{w,b,\zeta} \frac{1}{2} w^T w + C \sum_{i=1}^{n} \zeta_i$$
$$\text{subject to } y_i(w^T \phi(x_i) + b) \geq 1 - \zeta_i,$$
$$\zeta_i \geq 0, i = 1, \ldots, n$$

Intuitively, we're trying to maximize the margin (by minimizing $||w||^2 = w^T w$), while incurring a penalty when a sample is misclassified or within the margin boundary. Ideally, the value $y_i(w^T \phi(x_i) + b)$ would be ≥ 1 for all samples, which indicates a perfect prediction. But problems are usually not always perfectly separable with a hyperplane, so we allow some samples to be at a distance ζ_i from their correct margin boundary. The penalty term `C` controls the strength of this penalty, and as a result, acts as an inverse regularization parameter (see note below).

The dual problem to the primal is

$$\min_{\alpha} \frac{1}{2} \alpha^T Q \alpha - e^T \alpha$$
$$\text{subject to } y^T \alpha = 0$$
$$0 \leq \alpha_i \leq C, i = 1, \ldots, n$$

where e is the vector of all ones, and Q is an n by n positive semidefinite matrix, $Q_{ij} \equiv y_i y_j K(x_i, x_j)$, where $K(x_i, x_j) = \phi(x_i)^T \phi(x_j)$ is the kernel. The terms α_i are called the dual coefficients, and they are upper-bounded by C. This dual representation highlights the fact that training vectors are implicitly mapped into a higher (maybe infinite) dimensional space by the function ϕ: see kernel trick.

Once the optimization problem is solved, the output of decision_function for a given sample x becomes:

$$\sum_{i \in SV} y_i \alpha_i K(x_i, x) + b,$$

and the predicted class correspond to its sign. We only need to sum over the support vectors (i.e. the samples that lie within the margin) because the dual coefficients α_i are zero for the other samples.

These parameters can be accessed through the attributes `dual_coef_` which holds the product $y_i \alpha_i$, `support_vectors_` which holds the support vectors, and `intercept_` which holds the independent term b

Note: While SVM models derived from libsvm and liblinear use `C` as regularization parameter, most other estimators use `alpha`. The exact equivalence between the amount of regularization of two models depends on the exact objective function optimized by the model. For example, when the estimator used is **`Ridge`** regression, the relation between them is given as $C = \frac{1}{alpha}$.

▶ **LinearSVC**

▶ **NuSVC**

1.4.7.2. SVR

Given training vectors $x_i \in \mathbb{R}^p$, i=1,…, n, and a vector $y \in \mathbb{R}^n$ ε-SVR solves the following primal problem:

$$\min_{w,b,\zeta,\zeta^*} \frac{1}{2} w^T w + C \sum_{i=1}^{n} (\zeta_i + \zeta_i^*)$$
$$\text{subject to } y_i - w^T \phi(x_i) - b \leq \varepsilon + \zeta_i,$$
$$w^T \phi(x_i) + b - y_i \leq \varepsilon + \zeta_i^*,$$
$$\zeta_i, \zeta_i^* \geq 0, i = 1, \ldots, n$$

Here, we are penalizing samples whose prediction is at least ε away from their true target. These samples penalize the objective by ζ_i or ζ_i^*, depending on whether their predictions lie above or below the ε tube.

The dual problem is

$$\min_{\alpha,\alpha^*} \frac{1}{2} (\alpha - \alpha^*)^T Q (\alpha - \alpha^*) + \varepsilon e^T (\alpha + \alpha^*) - y^T (\alpha - \alpha^*)$$
$$\text{subject to } e^T (\alpha - \alpha^*) = 0$$
$$0 \leq \alpha_i, \alpha_i^* \leq C, i = 1, \ldots, n$$

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where e is the vector of all ones, Q is an n by n positive semidefinite matrix, $Q_{ij} \equiv K(x_i, x_j) = \phi(x_i)^T \phi(x_j)$ is the kernel. Here training vectors are implicitly mapped into a higher (maybe infinite) dimensional space by the function ϕ.

The prediction is:

$$\sum_{i \in SV} (\alpha_i - \alpha_i^*) K(x_i, x) + b$$

These parameters can be accessed through the attributes `dual_coef_` which holds the difference $\alpha_i - \alpha_i^*$, `support_vectors_` which holds the support vectors, and `intercept_` which holds the independent term b

▶ **LinearSVR**

1.4.8. Implementation details

Internally, we use libsvm [12] and liblinear [11] to handle all computations. These libraries are wrapped using C and Cython. For a description of the implementation and details of the algorithms used, please refer to their respective papers.

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